# Evaluation of ASOG Group Parameters for VLE of Systems Containing 1,4-Dioxane Mixtures

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Group contribution models such as UNIFAC and ASOG are frequently used to predict liquid phase activity coefficients for obtaining the vapor-liquid equilibria (VLE) of mixtures when no experimental data are available. To extend the applicability of group contribution models, it is important to define and increase new groups in addition to revising the values of group interaction parameters for improving the prediction accuracy.

Recent studies on the prediction of VLE of 1,4-dioxane containing systems indicate that the available published ASOG parameters are not adequate to give satisfactory predictions. To improve the prediction accuracy, a new group for 1,4-dioxane is defined and the interaction parameters are determined using the limited available binary experimental data. The VLE data, predicted from the new ASOG parameters, are compared with those predicted by the original and modified UNIFAC models.